Operator fidelity susceptibility: an indicator of quantum criticality

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We introduce an operator fidelity and propose to use its susceptibility for characterizing the sensitivity of quantum systems to perturbations. Two typical models are addressed: one is the transverse Ising model exhibiting a quantum phase transition, and the other is the one dimensional Heisenberg spin chain with next-nearest-neighbor interactions, which has the degeneracy. It is revealed that the operator fidelity susceptibility is a good indicator of quantum criticality regardless of the system degeneracy.

PACS numbers: 05.45.Mt; 03.65.Nk,03.65.Yz

Introduction—There are two important concepts, entanglement and fidelity in quantum information theory [1]. These two concepts are closely related to each other. For instance, fidelity, which was first proposed as a tool for describing the stability of a quantum system to perturbations [2], may be used to characterize quantum entanglement [3]. Notably, fidelity has recently been used to characterize quantum phase transitions (QPTs) [4, 5, 6, 7]. On the other hand, entanglement has also been employed to be an indicator of QPTs in many correlated quantum systems [8, 9, 10, 11].

How to characterize the stability of a quantum system to perturbations is an important issue as there is no quantum counterpart of the classical Lyapunov exponent. The Loshmidt echo [12] has been adopted as a measure of the system stability against perturbations, which is introduced as follows. Let operators U_0 and U_1 denote the time evolutions of Hamiltonians H_0 and H_1, where H_1 is slightly different from Hamiltonian H_0 with $H_1 - H_0 = \epsilon V$ as a small perturbation. In this case, the operator $U_{\rm e} = U_0^\dagger U_1$ is referred to as the echo operator, and the absolute value of its expectation over a specific state $|\psi\rangle$ is defined as the Loshmidt echo

$$L_{|\psi\rangle} = |\langle\psi|U_0^\dagger U_1|\psi\rangle|. \tag{1}$$

This is just the fidelity amplitude. Obviously, it is state-dependent, i.e., one has to choose an initial state (artificially in many cases) to evaluate its response to perturbations. This scenario to characterize QPT has a serious limitation, e.g., it can hardly be applied to a degenerated ground state, which has been a great challenge for a long time.

In this Letter, mainly motivated by the above challenge, we introduce a new kind of fidelity measure, called operator fidelity, and propose for the first time to use its susceptibility for characterizing the stability of quantum systems to perturbations. A distinct and significant merit lies in that it is state-independent and, in particular, is able to characterize the quantum criticality regardless of degeneracy. To illustrate the feasibility and reliability as well as the merit of the introduced operator fidelity susceptibility, here we employ it to investigate two typical QPT systems: the quantum Ising model and the Heisenberg model with next-nearest-neighbor interactions. Indeed, this fidelity susceptibility is able to serve as an indicator of QPT. In addition, for comparison, we also consider the mixed state fidelity susceptibility to address the quantum criticality with the ground-state degeneracy.

We begin with the definition of operator fidelity. Let $\mathcal{H}$ be a d-dimensional Hilbert space. All linear operators on $\mathcal{H}$ are represented by $d \times d$ matrices and thus their own may be considered to be vectors in an expanded d^2-dimensional Hilbert space $\mathcal{H}_{\rm HS}$. The inner product $\mathcal{H}_{\rm HS}$ is defined as the Hilbert-Schmidt product, i.e., for operators A and B, $\langle A|B\rangle = {\rm Tr}(A^\dagger B)$. In this sense, any linear operators on $\mathcal{H}$ can be considered as a state on $\mathcal{H}_{\rm HS}$. Thus, the fidelity of two states can naturally be generalized to the operator level. For two unitary evolution operators U_0 and U_1 on $\mathcal{H}$, the fidelity between them is defined as

$$F^2 = \frac{1}{d^2}|{\rm Tr}(U_0^\dagger U_1)|^2 = |\overline{\rm Tr}(U_0^\dagger U_1)|^2, \tag{2}$$

where the averaged tracing operation is defined as $\overline{\rm Tr}\,() = {\rm Tr}()\,/d$. It is notable that one may obtain the averaged Loshmidt echo [13]-[16] after averaging $L_{|\psi\rangle}$ over all states on $\mathcal{H}$ with a Haar measure, and the averaged Loschmidt echo and the operator fidelity are essentially equivalent. Remarkably, the operator fidelity involves not only the ground state, but also all eigenstates of the system. It quantifies the difference between two unitary operators, and is a conserved quantity under local operation in Hilbert space $\mathcal{H}_{\rm HS}$.

We can rewrite the echo operator $U_{\rm e}$ as [17]

$$U_{\rm e} \;=\; 1 - i\epsilon\int_0^t V_I(t_1)dt_1$$

$$-\epsilon^2 \int_0^t \int_0^{t_1} V_I(t_1) V_I(t_2) dt_1 dt_2 + O(\epsilon^3), \quad (3)$$

where $V_I(t) = \exp(iH_0 t) V(t) \exp(-iH_0 t)$ is the perturbation operator in the interaction picture. After tracing, we have

$$\overline{\mathrm{Tr}}(U_{\mathrm{e}}) = 1 - i\epsilon \overline{\mathrm{Tr}}[W(t)] - \frac{\epsilon^2}{2} \overline{\mathrm{Tr}}[W(t)^2] + O(\epsilon^3), \quad (4)$$

where $W(t) = \int_0^t V_I(t') dt'$. Then from Eq.(2), we obtain

$$F^2 = 1 - \epsilon^2 [\overline{\mathrm{Tr}}(W(t)^2) - \overline{\mathrm{Tr}}^2(W(t))] + O(\epsilon^4). \quad (5)$$

To evaluate the above operator fidelity, one has to choose a small parameter artificially, which is ϵ-dependent. To avoid this artifact, we can also introduce a so-called fidelity susceptibility [4, 18], which is given by

$$\chi_F = \lim_{\epsilon \to 0} \frac{1-F}{\epsilon^2} = \frac{1}{2} \{ \overline{\mathrm{Tr}} \left[W(t)^2 \right] - \overline{\mathrm{Tr}}^2 \left[W(t) \right] \}. \quad (6)$$

Remarkably, the above simple formula possesses a distinct computational advantage that enables one to calculate straightforwardly the fidelity susceptibility from $W(t)$, which can also be evaluated readily or at least numerically for more complicated systems. On the other hand, generally speaking, a quantity/measure susceptibility responds to the relevant perturbations more sensitively than the quantity/measure itself does, so we believe that it could capture a drastic change feature of the quantum evolution (versus the relevant parameter) around a critical point. We below explore the intriguing relationship between the operator fidelity susceptibility and the QPT in two typical systems, with one having degeneracy.

Quantum phase transition—The first system we consider is an Ising spin chain subject to a transverse magnetic field, whose Hamiltonian reads

$$H_0 = \sum_{l=-M}^{M} \left(\sigma_l^x \sigma_{l+1}^x + \lambda \frac{\sigma_l^z}{2} \right), \quad (7)$$

where λ characterizes the strength of the transverse field, σ_l^α $(\alpha = x, y, z)$ are the Pauli operators defined on the l-th site, and the total number of spins in the Ising chain is $N = 2M+1$. The perturbation operator is given by $\epsilon V = \epsilon \sum_{l=-M}^{M} \sigma_l^z / 2$. There are two competing terms in the Hamiltonian, i.e, the Ising interaction and the transverse field term.

The Hamiltonian can be diagonalized by combining Jordan-Wigner transformation and Fourier transformation to the momentum space, i.e.,

$$H_0 = \sum_{k>0} e^{i\frac{\theta_k}{2}\sigma_{kx}} \left(\Omega_k \sigma_{kz} \right) e^{-i\frac{\theta_k}{2}\sigma_{kx}} + \left(1 - \frac{\lambda}{2} \right) \sigma_{0z} \quad (8)$$

where we have used the following pseudospin operators $\sigma_{k\alpha}\,(\alpha = x, y, z)$: $\sigma_{kx} = d_k^\dagger d_{-k}^\dagger + d_{-k} d_k, (k = 1, 2, ...M), \sigma_{ky} = -i d_k^\dagger d_{-k}^\dagger + i d_{-k} d_k, \sigma_{kz} = d_k^\dagger d_k + d_{-k}^\dagger d_{-k} - 1, \sigma_{0z} = 2 d_0^\dagger d_0 - 1$. Operators $d_k^\dagger, d_k \{k = 1, 2, ...M\}$ denote the fermionic creation and annihilation operators in the momentum space. Here,

$$\begin{aligned} \Omega_k &= \sqrt{\left[-\lambda + 2\cos\left(\frac{2\pi k}{N} \right) \right]^2 + 4\sin^2\left(\frac{2\pi k}{N} \right)}, \\ \theta_k &= \arcsin\left[\frac{-2\sin\left(\frac{2\pi k}{N}\right)}{\Omega_k} \right]. \end{aligned} \quad (9)$$

Then the time evolution operator is derived as (with $\hbar = 1$)

$$U_0(t) = e^{-i(-\frac{\lambda}{2}+1)\sigma_{0z} t} \prod_{k>0} e^{i\frac{\theta_k}{2}\sigma_{kx}} e^{-it\Omega_k \sigma_{kz}} e^{-i\frac{\theta_k}{2}\sigma_{kx}}. \quad (10)$$

The unitary operator $U_1(t)$ for Hamiltonian $H_1 = H_0 + \epsilon V$ can be obtained by just replacing λ with $\lambda + \epsilon$ in the above equation.

At this stage, from $U_0(t)$ and $U_1(t)$ given above, we are able to obtain $W(t)$ as,

$$\begin{aligned} W(t) &= \sum_{k>0} [\sigma_{kz} \left(t\cos^2\theta_k + \frac{\sin^2\theta_k}{2\Omega_k} \sin 2t\Omega_k \right) \\ &\quad + \sigma_{ky} \cos\theta_k \sin\theta_k \left(t - \frac{1}{2\Omega_k} \sin 2t\Omega_k \right) \\ &\quad + \sigma_{kx} \sin\theta_k \frac{1}{2\Omega_k} \left(\cos 2t\Omega_k - 1 \right)] + \frac{t}{2}\sigma_{0z} \end{aligned} \quad (11)$$

Consequently, the fidelity susceptibility is derived exactly

$$\begin{aligned} \chi_F &= \frac{1}{2} t^2 \left(\frac{1}{2} + \sum_{k>0} \cos^2\theta_k \right) \\ &\quad + \frac{1}{2} \sum_{k>0} \sin^2(\Omega_k t) \sin^2\theta_k / \Omega_k^2. \end{aligned} \quad (12)$$

Note that the first term in Eq. (12), which is proportional to the square of time t, plays a dominant role when t is large.

In the transverse Ising model, two phases are separated by the quantum phase transition point $\lambda = 2$. The singular behavior of QPT at the transition point reflects the sensitivity of ground state to perturbations. At this stage, we numerically look into the behaviors of the operator fidelity susceptibility and its partial derivative with respect to λ at a finite time $t = 100$ (the natural units are used here). As shown in Fig. 1 for different system sizes, the transition point is unambiguously signatured: it is clearly seen that the fidelity susceptibility and its partial derivative are nearly unchanged when increasing λ from 0 to 2; the derivative increases sharply at the transition point and the derivative peak is higher when the system size becomes larger.

The behavior of the operator fidelity susceptibility at the QPT point is different from that of the ground-state

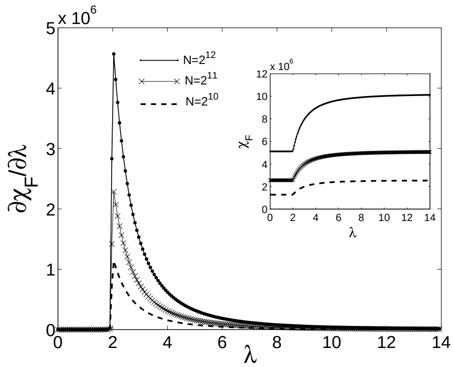

FIG. 1: Partial derivative of the fidelity susceptibility versus the parameter λ for different system sizes $N = 2^{10}, 2^{11}, 2^{12}$. The insert plots the fidelity susceptibility χ_F versus the parameter λ. The time $t = 100$.

fidelity [4]. The ground-state fidelity susceptibility displays a sudden increase at the QPT point, reflecting the drastic change of ground state of the system when the QPT occurs, while the operator fidelity susceptibility drops to a certain value continuously at the QPT point(and is unchanged below the point) since it involves the all eigenstates and characterizes the sensitivity of the whole system to perturbations in the time evolution. However, on the other hand, its partial derivative changes discontinuously at the QPT point and is much more sensitive to perturbations, being able to single out the QPT point unambiguously.

Heiserberg model with next-nearest-neighbor interactions—For the fidelity scenario developed previously for QPTs, only pure ground states can be addressed, without taking into account the degeneracy; while it is the case for some quantum systems. As seen above, the operator fidelity approach has an advantage that the degeneracy is not necessary to be considered explicitly. To contrast our approach with the state fidelity approach, we below address a model with the ground-state degeneracy. The Hamiltonian of one-dimensional Heisenberg system with next-nearest-neighbor interaction reads

$$H_0 = \sum_{i}^{N} \left(J_1 \mathbf{s}_i \cdot \mathbf{s}_{i+1} + J_2 \mathbf{s}_i \cdot \mathbf{s}_{i+2} \right), \tag{13}$$

where the $\mathbf{s}_i$ denotes the spin-1/2 operator at the i_{th} site, N is the total number of sites, J_1 and J_2 are the nearest-neighbor (NN) and next-nearest-neighbor (NNN) exchange couplings. As usual, we choose the periodic boundary condition and set $J_1 = 1$ for convenience. The perturbation operator is given by $\epsilon V = \epsilon \sum_i \mathbf{s}_i \cdot \mathbf{s}_{i+2}$. Note that no exact analytical results are available for this model (13) except the special case of $J_2 = 0$ and $J_2 = 1/2$.

It is well known that the point $J_2 = 1/2$ corresponds to the Majumdar-Ghosh model where the ground state is the products of dimers, leading to a gaped phase [21].

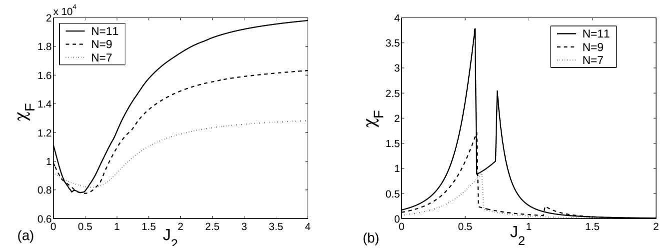

FIG. 2: (a) The operator fidelity susceptibility versus J_2 for different system sizes $N = 7, 9, 11$. (b) The mixed state fidelity susceptibility versus J_2.

Chen *et al* [22] studied the ground-state fidelity and first-excited-state fidelity of this system with even number of sites. Here we focus on the odd number of sites as the fourfold degenerate energy level structure is present in this case.

We first diagonalize the Hamiltonians numerically, and then calculate the operator fidelity susceptibility versus the NNN coupling J_2 for $N = 7, 9, 11$, as plotted in Fig. 2(a). At a finite time $t = 100$, the susceptibility χ_F decays to a minimum value near the critical point $J_2 = 0.5$. With the size increasing, the minimum point is closer to the critical point. It is expected that the curve around the minimum point would become sharper and sharper when the size increases, leading to a discontinuity in its partial derivative with respect to J_2 at the critical point in the thermodynamic limit, as in the case of the transverse Ising system. We indeed note from the energy spectrum that the ground energy level and the excited energy level crosses near the point $J_2 = 0.5$. In this sense, the operator-fidelity susceptibility (or its partial derivative) is also able to capture the level crossing feature in the system and thus to indicate the critical point, overcoming the subtle problem induced by the degeneracy.

On the other hand, at least for comparison, it is also interesting to consider an alternative approach to address degenerate cases by making use of the mixed state fidelity given by [23]

$$F(\rho_0, \rho_1) \equiv \mathrm{Tr}\left(\sqrt{\rho_1^{1/2} \rho_0 \rho_1^{1/2}}\right) = \mathrm{Tr}\left(\sqrt{\rho_0 \rho_1}\right). \tag{14}$$

Without loss of generality, it is not unreasonable to assume the mixed ground state as an equal mixture of the degenerate ground states,

$$\rho_j = \frac{1}{R} \sum_{r=1}^{R} \left| \psi_{jr} \right\rangle \left\langle \psi_{jr} \right|, \tag{15}$$

with $r = 1, 2, ...R$ denote the degeneracy and the state $|\psi_{jr}\rangle$ denotes the j_{th} degenerate eigenstate of the system. In the fidelity $F(\rho_0, \rho_1)$ of this Heisenberg spin chain with the NNN interactions, ρ_0 comes from the mixture of the ground states of H_0, and ρ_1 corresponds to $H_1 = H_0 + \epsilon V$.

When the degeneracy of the system is explicitly obtained, we evaluate the mixed state fidelity susceptibility versus the coupling strength J_2 by combining Eq.(6) with Eq. (14), as shown in Fig. 2(b). Clearly, the susceptibility χ_F passes the critical point $J_2 = 0.5$ discontinuously. For larger sizes such as $N = 9, 11$, there exist two peaks since the ground energy level crossing occurs twice. With increasing the system size, the position of the first peak approaches to the critical point, and the second one is closer to the first one. Although, it seems that the suggested mixed state fidelity approach may also indicate the critical point, it should be pointed out that it is feasible only when the degeneracy of the ground states is explicitly known and the equal mixture of the degenerated states is assumed. In addition, due to the energy level crossing, the degeneracy may change at the critical point and thus the mixed state fidelity approach may not be workable for all the values of the considered parameter.

Relationship to entangling power—Finally, we would like to disclose an intrinsic connection between the present operator fidelity and the entangling power [19] that was adopted to characterize the entangling capability of a quantum evolution. The entangling power is essentially the mean state linear entropy at time t after averaging over all initial states. We consider a general Hamiltonian in the form

$$H = I \otimes H_0 + |1\rangle\langle 1| \otimes V = |0\rangle\langle 0| \otimes U_0 + |1\rangle\langle 1| \otimes H_1, \quad (16)$$

where I is the identity operator and $H_1 = H_0 + V$. The time evolution operator is readily obtained as $U(t) = |0\rangle\langle 0| \otimes U_0(t) + |1\rangle\langle 1| \otimes U_1(t)$, where $U_k(t) = \exp(-iH_k t)\{k = 0, 1\}$. This is a kind of the controlled-U operator, for which the entangling power e_{p} is proportional to the operator entanglement $E[U(t)]$ [20], i.e., $e_{\mathrm{p}}[U(t)] = [d/(d+1)]^2 E[U(t)]$. The operator entanglement $E[U(t)]$ can be straightforwardly obtained from the expression of $U(t)$. Finally, we obtain

$$e_{\mathrm{p}} = \frac{d^2}{2(d+1)^2}[1 - F^2]. \quad (17)$$

This establishes a direct connection between the entangling power and operator fidelity.

Summary— We have proposed an operator fidelity approach to characterize the stability of quantum system to perturbations, which possesses a remarkable advantage that it is state-independent and is able to characterize the quantum criticality regardless of degeneracy. We have employed the approach to reveal successfully the QPT points in two typical systems: the quantum Ising model and the Heisenberg chain with next-nearest-neighbor interactions, with the latter having the degeneracy. Our approach is quite promising for the exploration of quantum instability including QPT and quantum chaos.

Acknowledgements The authors would like to thank C. P. Sun, S. J. Gu, and P. Zanardi for their helpful discussions. The work was supported by the Program for New Century Excellent Talents in University (NCET), the NSFC with grant nos. 90503003 and 10429401, the State Key Program for Basic Research of China with grant nos. 2006CB921206 and 2006CB921800, the Specialized Research Fund for the Doctoral Program of Higher Education with grant No.20050335087, and the RGC grants (HKU7045/05P and HKU7049/07P).

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